Notes on Canonical Transformation

For a given quantum system, sometimes we are only interested in the effective Hamiltonian in a reduced Hilbert space which is a partial set of the original space. This is usefully to simplify the problem in the limit of certain parameters. For instance, the Kondo limit of the Anderson impurity problem, where the single occupancy of the impurity level is assumed while the charge fluctuations are neglected.

Technically, we can find a canonical transformation(CT) to map the original Hamiltonian into an effective Hamiltonian in a reduced Hilbert space. A general canonical transformation is defined as

$$H_{can} = e^S H e^{-S} = H + [S, H] + \frac{1}{2}[S, [S, H]] + \frac{1}{3!}[S, [S, [S, H]]] + \dots . \tag{1}$$

and it consists of three steps,

- Separate the Hamiltonian into two parts,

  $$H = H_0 + H_m, \tag{2}$$

  where H_m contains all terms which mix the states in reduced Hilbert space and the rest.

- Find a transformation S to eliminate the mixing terms H_m. This can be carried out order by order. For instance, the first order, we pick S to satisfy

  $$[H_0, S^{(1)}] = H_m. \tag{3}$$

- Since all terms mixing the reduced Hilbert space and rest are eliminated, we can simply use a projection operator to project out the unwanted states.

I. LIOUVILLE OPERATORS

Liouville operators are defined as $L_x A = [H_x, A]$. The transformation then can be easily express as

$$S^{(1)} = \frac{1}{L_0} H_m. \tag{4}$$

Some properties of the Liouville operators are

$$(La)^\dagger = -[H, a^\dagger] = -La^\dagger$$
$$(La)^\dagger = (\lambda a)^\dagger = \lambda^* a^\dagger. \tag{5}$$

II. HUBBARD OPERATORS

The complete Hilbert space for an electron (spin 1/2 fermion) in a quantum state consists of four states: zero occupancy, spin-up, spin-down, double occupancy. It is usually to introduce Hubbard operators $X_i^{ab} = |a\rangle_{ii}\langle b|$.

The electron creation/annihination operators can be expressed as

$$\begin{aligned} f_{i\sigma}^\dagger &= X_i^{\sigma 0} + \eta(\sigma) X_i^{d\bar{\sigma}} \\ f_{i\sigma} &= X_i^{0\sigma} + \eta(\sigma) X_i^{\bar{\sigma}d} \end{aligned} \tag{6}$$

where $\eta(\sigma) = \pm 1$, for $\sigma = \pm 1/2$, while in reverse the Hubbard operators can be written as

$$X^{00} = (1 - n_\uparrow)(1 - n_\downarrow) \tag{7}$$
$$X^{\sigma\sigma} = n_\sigma (1 - n_{\bar{\sigma}}) \tag{8}$$
$$X^{dd} = n_\uparrow n_\downarrow \tag{9}$$
$$X^{\sigma 0} = f_\sigma^\dagger (1 - n_{\bar{\sigma}}) \tag{10}$$
$$X^{d\sigma} = \eta(\bar{\sigma}) f_{\bar{\sigma}}^\dagger n_\sigma \tag{11}$$
$$X^{d0} = f_\uparrow^\dagger f_\downarrow^\dagger \tag{12}$$
$$X^{\sigma\bar{\sigma}} = f_\sigma^\dagger f_{\bar{\sigma}} \tag{13}$$

Some properties of the Hubbard operators are

$$[X_i^{ab}, X_j^{cd}] = \delta_{ij}(\delta_{bc} X_i^{ad} - \delta_{da} X_i^{cb}) \tag{14}$$
$$(X^{ab})^\dagger = X^{ba} \tag{15}$$

Comment: the first relation only holds for boson-like operators between sites to apply δ_{ij}, for instance $X^{\sigma\bar{\sigma}}$.

III. EXAMPLE: MAPPING THE ANDERSON LATTICE MODEL INTO KONDO LATTICE MODEL

This is a generalization of Schrieffer-Wolf transformation to single impurity problem, while can be adapted into a few impurity problems.

The Anderson lattice model consists of f-electrons (on each lattice sites) embedded in a conduction electron band,

$$
\begin{aligned}
H_{ALM} &= H_c + H_f + H_{c-f} \\
H_c &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \qquad (16) \\
H_f &= \sum_i \left[\sum_\sigma \epsilon_{fi\sigma} n_{fi\sigma} + U_i n_{fi\uparrow} n_{fi\downarrow} \right] \\
H_{c-f} &= \sum_i \sum_\sigma \left(v_{ik} e^{i\mathbf{k}\cdot\mathbf{r}_i} f^\dagger_{i\sigma} c_{k\sigma} + H.c. \right). \qquad (17)
\end{aligned}
$$

We are interested in the effective Hamiltonian with single occupancy states on each site only. Therefore, we identify $H_m = H_{c-f}$ and $H_0 = H_c + H_f$.

With Hubbard operators we rewrite the Hamiltonian as

$$
\begin{aligned}
H_f &= \sum_{i\sigma} \epsilon_{fi} X_i^{\sigma\sigma} + \sum_i (2\epsilon_{fi} + U_i) X_i^{dd} \\
H_{c-f} &= \sum_{i\sigma} \left\{ v_{ik} e^{i\mathbf{k}\cdot\mathbf{r}_i} \left(X_i^{\sigma 0} + \eta(\sigma) X_i^{d\bar{\sigma}} \right) c_{\mathbf{k}\sigma} + v^*_{ik} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c^\dagger_{k\sigma} \left(X_i^{0\sigma} + \eta(\sigma) X_i^{\bar{\sigma} d} \right) \right\} \qquad (18)
\end{aligned}
$$

The first order of the transformation is to make

$$
[H_c + H_f, S^{(1)}] = H_{c-f}. \qquad (19)
$$

or $S^{(1)} = \frac{1}{L_c + L_f} H_{c-f}$ with the Liouville operator $L_x A = [H_x, A]$. We find that

$$
\begin{aligned}
S^{(1)} = \sum_{i\sigma} \Bigg\{ & v_{ik} e^{i\mathbf{k}\cdot\mathbf{r}_i} \left(X_i^{\sigma 0} c_{\mathbf{k}\sigma} \frac{1}{-\epsilon_k + \epsilon_{fi}} + \eta(\sigma) X_i^{d\bar{\sigma}} c_{\mathbf{k}\sigma} \frac{1}{-\epsilon_k + \epsilon_{fi} + U_i} \right) \\
& + v^*_{ik} e^{-i\mathbf{k}\cdot\mathbf{r}_i} \left(c^\dagger_{k\sigma} X_i^{0\sigma} \frac{1}{\epsilon_k - \epsilon_{fi}} + \eta(\sigma) c^\dagger_{k\sigma} X_i^{\bar{\sigma} d} \frac{1}{\epsilon_k - \epsilon_{fi} - U_i} \right) \Bigg\} \qquad (20)
\end{aligned}
$$

and the effective Hamiltonian is

$$
H^{(1)}_{can} = \frac{1}{2} [S^{(1)}, H_{c-f}]. \qquad (21)
$$

Onsite terms are

$$
\begin{aligned}
H^{(1)a} &= \frac{1}{2}\sum_{i,k,k',\sigma} v_{ik}v_{ik'}e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}_i}\eta(\sigma)X_i^{d0}c_{k\sigma}c_{k'\bar{\sigma}}\left(\frac{1}{-\epsilon_k+\epsilon_f}+\frac{1}{-\epsilon_k+\epsilon_f+U_i}\right)\\
&+ \frac{1}{2}\sum_{i,k,k',\sigma} v^*_{ik}v^*_{ik'}e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}_i}\eta(\sigma)X_i^{0d}c^\dagger_{k\sigma}c^\dagger_{k'\bar{\sigma}}\left(\frac{1}{-\epsilon_k+\epsilon_f}+\frac{1}{-\epsilon_k+\epsilon_f+U_i}\right)\\
H^{(1)b} &= \frac{1}{2}\sum_{i,k,k',\sigma,\sigma'} v_{ik}v^*_{ik'}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i}c_{k\sigma}c^\dagger_{k'\sigma'}\left(\frac{X_i^{\sigma\sigma'}-X_i^{00}\delta_{\sigma\sigma'}}{-\epsilon_k+\epsilon_f}+\eta(\sigma)\eta(\sigma')\frac{X_i^{dd}\delta_{\sigma\sigma'}-X_i^{\bar{\sigma}'\bar{\sigma}}}{-\epsilon_k+\epsilon_f+U_i}\right)\\
&+ \frac{1}{2}\sum_{i,k,k',\sigma,\sigma'} v^*_{ik}v_{ik'}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i}c^\dagger_{k\sigma}c_{k'\sigma'}\left(\frac{X_i^{\sigma'\sigma}-X_i^{00}\delta_{\sigma\sigma'}}{-\epsilon_k+\epsilon_f}+\eta(\sigma)\eta(\sigma')\frac{X_i^{dd}\delta_{\sigma\sigma'}-X_i^{\bar{\sigma}\bar{\sigma}'}}{-\epsilon_k+\epsilon_f+U_i}\right)
\end{aligned}
\tag{22}
$$

$H^{(1)a}$ is to be cancelled in the next order. For $H^{(1)b}$, we project out empty and double occupancy states, for instance, terms containing d or 0. The terms lefts are rearranged into Kondo coupling and potential scattering terms on each site.

$$
H^{(1)}_{eff} = \sum_i e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i}\left(J_{i,k,k'}c^\dagger_{k\alpha}\vec{\sigma}_{\alpha\beta}c_{k'\beta}\cdot\mathbf{S}_i + V_{i,k,k'}c^\dagger_{k\alpha}c_{k'\alpha}\right). \tag{23}
$$

For intersite terms, those with $[X_ic_{k\sigma}, X_jc^\dagger_{k'\sigma'}] = X_iX_j\delta_{k,k'}\delta_{\sigma,\sigma'}$ combinations will survive.

$$
\begin{aligned}
H^{(1)c} &= \frac{1}{2}\sum_{i\neq j}\left\{\sum_{k\sigma} v_{ik}v^*_{jk}e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\left(X_i^{\sigma0}X_j^{0\sigma}+\eta(\sigma)X_i^{\sigma0}X_j^{\bar{\sigma}d}\right)\frac{1}{-\epsilon_k+\epsilon_{fi}}\right.\\
&+\sum_{k\sigma} v_{ik}v^*_{jk}e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\left(\eta(\sigma)X_i^{d\bar{\sigma}}X_j^{0\sigma}+X_i^{d\bar{\sigma}}X_j^{\bar{\sigma}d}\right)\frac{1}{-\epsilon_k+\epsilon_{fi}+U_i}\\
&+\sum_{k\sigma} v^*_{ik}v_{jk}e^{-i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\left(X_i^{0\sigma}X_j^{\sigma0}+\eta(\sigma)X_i^{0\sigma}X_j^{d\bar{\sigma}}\right)\frac{1}{\epsilon_k-\epsilon_{fi}}\\
&\left.+\sum_{k\sigma} v^*_{ik}v_{jk}e^{-i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\left(\eta(\sigma)X_i^{\bar{\sigma}d}X_j^{\sigma0}+X_i^{\bar{\sigma}d}X_j^{d\bar{\sigma}}\right)\frac{1}{\epsilon_k-\epsilon_{fi}-U_i}\right\}
\end{aligned}
\tag{24}
$$

(The third and fourth terms are h.c. of the first and second terms, respectively.) Notice that $X_i^{\sigma0}X_j^{0\sigma}+\eta(\sigma)X_i^{\sigma0}X_j^{\bar{\sigma}d} = f^\dagger_{i\sigma}f_{j\sigma}(1-n_{j\bar{\sigma}})$ and $\eta(\sigma)X_i^{d\bar{\sigma}}X_j^{0\sigma}+X_i^{d\bar{\sigma}}X_j^{\bar{\sigma}d} = f^\dagger_{i\sigma}f_{j\sigma}n_{i\bar{\sigma}}$. These correspond to direct f-hopping terms. Of course, if we enforce the single occupancy on each site, i.e., only terms as $X_i^{\sigma\sigma'}X_j^{\sigma"\sigma'''}$ are allowed, these terms are to be eliminated.